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ADAPTIVE FINITE ELEMENT METHOD III: MESH REFINEMENT

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An adaptive finite element method is developed to solve initial boundary value problems for vector systems of parabolic partial differential equations in one space dimension and time. The differential equations are discretized in space using piecewise linear finite element approximations. Superconvergence properties and quadratic polynomials are used to derive a computationally inexpensive approximation to the spatial component of the error. This technique is coupled with time integration schemes of successively higher orders to obtain an approximation of the temporal and total discretization errors. The approximate errors are used to control an adaptive mesh refinement strategy. Refinement is performed in space, time, or both space and time depending on the dominant component of the error estimate. Levels of refinement are determined automatically based on the theoretical orders of the numerical methods. Computational results provide an indication of the utility of such a strategy in keeping the total error within a prescribed tolerance.

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INTRODUCTION

This is the third in a series of four reports whose overall purpose is to describe an adaptive finite element method (AFEM) for solving systems of parabolic partial differential equations. In particular, AFEM attempts to find a numerical solution of an M-dimensional system of the form

$$\boldsymbol{u}_t(x,t) + \boldsymbol{f}(x,t,\boldsymbol{u},\boldsymbol{u}_x) = [\boldsymbol{D}(x,t,\boldsymbol{u})\boldsymbol{u}_x(x,t)]_x \ , \ a<x<b \ , \ t>0 \ , \tag{1a}$$

subject to the initial conditions

$$\boldsymbol{u}(x,0) = \boldsymbol{u}^0(x) \ , \ a \le x \le b \tag{1b}$$

and linear separated boundary conditions

$$\begin{aligned} \boldsymbol{A}^l(t)\boldsymbol{u}(a,t) + \boldsymbol{B}^l(t)\boldsymbol{u}_x(a,t) &= \boldsymbol{g}^l(t) \\ \boldsymbol{A}^r(t)\boldsymbol{u}(b,t) + \boldsymbol{B}^r(t)\boldsymbol{u}_x(b,t) &= \boldsymbol{g}^r(t) \end{aligned} \ , \ t>0 \ . \tag{1c}$$

The variables x and t represent spatial and temporal coordinates and denote partial differentiation when they are used as subscripts; $\boldsymbol{u}$, $\boldsymbol{f}$, $\boldsymbol{u}^0$, $\boldsymbol{g}^l$, and $\boldsymbol{g}^r$ are M-vectors; and $\boldsymbol{D}$, $\boldsymbol{A}^l$, $\boldsymbol{B}^l$, $\boldsymbol{A}^r$, and $\boldsymbol{B}^r$ are $M \times M$ matrices.

The problem is assumed to be well-posed and parabolic; thus, e.g., $\boldsymbol{D}(x,t,\boldsymbol{u})$ is positive definite. The rows of $\boldsymbol{B}^l$ and $\boldsymbol{B}^r$ are restricted to be either entirely zero or a row of the $M \times M$ identity matrix. When the i^{th} row of $\boldsymbol{B}^l$ or $\boldsymbol{B}^r$ is identically zero, then A^l_{ii} or A^r_{ii} cannot be zero, respectively, and the boundary condition is a Dirichlet (essential) condition. Otherwise, the boundary condition is a Neumann or Robbins (natural) condition. The ultimate goal of AFEM is to determine an approximate solution to Eq. (1) to within a user prescribed error tolerance.

The adaptive strategies utilized by AFEM are: (1) error estimation, coupled with (2) local mesh refinement (cf., e.g., Adjerid and Flaherty (ref 1), Babuska and Dorr (ref 2), Babuska, Zienkiewicz, Gago, and Oliveira (ref 3), Bank and Weiser (ref 4), Berger and Oliger (ref 5), Bieterman and Babuska (refs 6,7), Moore and Flaherty (ref 8), Shephard (ref 9), Strouboulis and Oden (ref 10), Zienkiewicz and Zhu (ref 11)), and (3) mesh movement (cf., e.g., Adjerid and Flaherty (ref 1), Arney and Flaherty (ref 12), Bell and Shubin (ref 13), Davis and Flaherty (ref 14), Dorfi and Drury (ref 15), Dwyer (ref 16), Ewing, Russell, and Wheeler (ref 17), Hyman (ref 18), Kansa, Morgan, and Morris (ref 19), Miller and Miller (refs 20,21), Petzold (ref 22), Rai and Anderson (ref 23), Russell and Ren (ref 24), Saltzman and Brackbill (ref 25), Smooke and Koszykowski (ref 26), Thompson (ref 27), Verwer, Blom, Furzeland, and Zegeling (ref 28), and White (ref 29)).

The purpose of this report is to describe the mesh refining procedures employed by AFEM. Detailed summaries of how AFEM implements its other adaptive strategies are found in separate reports entitled: Adaptive Finite Element Method II: Error Estimation (ref 30) and Aadaptive Finite Element Method IV: Mesh Movement (ref 31). Furthermore, the report, Adaptive Finite Element Method I: Solution Algorithm and Computational Examples (ref 32),

describes how all the adaptive algorithms are implemented in unison and contains results demonstrating the utility of AFEM as a computational tool. However, to fully understand how and why AFEM performs mesh refinement, a brief description of its error estimating procedures is presented here since error estimation controls the mesh refinement (cf., Coyle and Flaherty (ref 30) for a more detailed account).

Two main error-controlled adaptive finite element techniques for parabolic partial differential equations (PDEs) have evolved. One technique is a method of lines (MOL) (cf., e.g., Adjerid and Flaherty (ref 1) and Bieterman and Babuska (refs 6,7)) approach that uses a Galerkin method to discretize the PDEs in space and one of the many excellent ordinary differential equations (ODEs) solvers (cf., e.g., Gear (ref 33) and Petzold (ref 34)) to integrate in time. Spatial elements are added and deleted in regions of high and low error when deemed necessary, and all elements are advanced in time according to the ODE solver. The second technique is a local refinement method (LRM) (cf., e.g., Berger and Oliger (ref 5) and Moore and Flaherty (ref 8)) that uses Galerkin approximations and/or finite difference techniques in both space and time. Fine grids of space-time elements are added to coarser grids, and the problem is recursively solved in regions of high error.

The strategy developed here is an MOL technique with features of an LRM which attempts to take advantage of the strengths of both methods. The basic idea is to divide the total error into its spatial and temporal components (cf., Coyle and Flaherty (ref 30)). Using these various error estimates, one can then decide on the type of refinement that is needed: spatial, temporal, or both. MOL only refines in space, while maintaining the temporal error tolerance at a fraction of the spatial error (cf., e.g., Adjerid and Flaherty (ref 1) and Bieterman and Babuska (refs 6,7)). Developers of LRM, on the other hand, control the total error by simultaneous refinement in space and time (cf., Berger and Oliger (ref 5)). As a result, both methods can do more work than necessary.

Our algorithm is an MOL approach with the added ability to "back track" and solve the problem again with a finer discretization. Back tracking is usually associated with an LRM, although some MOL's codes now include it (cf., Adjerid and Flaherty (ref 1)). Spatial refinement is performed locally using the spatial error estimate to determine the location and degree of refinement. Temporal refinement is global using the temporal error estimate to determine an improved time step. The problem is solved again whenever refinement is necessary by advancing the entire spatial solution in time with the appropriate time step.

This strategy, like MOL but unlike LRM, avoids artificial internal boundaries and complicated data structures since there is no need to keep track of layers upon layers of refined space-time grids as well as the solutions on those grids (cf., e.g., Berger and Oliger (ref 5) and Moore and Flaherty (ref 8)). However, like LRM, this strategy utilizes the fact that the ODEs arise from discretizing a PDE, and since this strategy has the ability to back track, it is more difficult to deceive and less sensitive to coarse grid selection (cf., e.g., Adjerid and Flaherty (ref 1), Berger and Oliger (ref 5), and Moore and Flaherty (ref 8)).

In order to obtain an approximate solution and the various error estimates mentioned above, AFEM discretizes Eq. (1a) in space using Galerkin's method with piecewise linear finite elements. Temporal discretization is performed by the backward Euler method. A second solution is calculated using trapezoidal rule integration in time, and the difference between the

two solutions is used to furnish an estimate of the temporal discretization error. A third solution is obtained using quadratic finite elements and the trapezoidal rule in time. This solution is higher order in space and time than the original piecewise linear finite element-backward Euler solution. Hence, it can be used to provide an estimate of the total discretization error of the piecewise linear finite-element backward Euler solution. Furthermore, the difference between the piecewise linear and quadratic solutions calculated by the trapezoidal rule furnishes an estimate of the spatial discretization error (cf., Moore and Flaherty (ref 8) or Coyle and Flaherty (ref 35)).

AFEM's goal is to estimate the discretization error per time step in solutions obtained by using piecewise linear finite element approximations in space and the backward Euler method in time. It seems most appropriate to gage errors in the H^1 norm

$$\|e\|_1 = [(e_x,e_x) + (e,e)]^{1/2} ; \tag{2}$$

however, other metrics may also be used. An error estimate that is global in space and local in time may at first seem unusual, but it is commonly used when spatial finite element approximations are combined with temporal finite difference methods (cf., Thomée (ref 36)).

Let the piecewise linear finite element solutions at time t^n obtained by using backward Euler and trapezoidal rule temporal integration be denoted by U_1^n and $U_{1/2}^n$, respectively. Likewise, let $\hat{U}_{1/2}^n$ denote the piecewise quadratic finite element solution at t^n found by using the trapezoidal rule integration in time.

It is known (cf., Strang and Fix (ref 37)) that

$$\|u(\cdot,t^n) - U_1^n(\cdot)\|_1 = O((\Delta t^n)^2) + O(N^{-1}) . \tag{3}$$

Since

$$\|u(\cdot,t^n) - \hat{U}_{1/2}^n(\cdot)\|_1 = O((\Delta t^n)^3) + O(N^{-2}) , \tag{4}$$

one should be able to use the difference between $\hat{U}_{1/2}^n$ and U_1^n to estimate the error in U_1^n ; thus,

$$\begin{aligned} \|u - U_1^n\|_1 &\le \|\hat{U}_{1/2}^n - U_1^n\|_1 + \|u - \hat{U}_{1/2}^n\|_1 \\ &\le \|\hat{U}_{1/2}^n - U_1^n\|_1 + O((\Delta t^n)^3) + O(N^{-2}) . \end{aligned} \tag{5}$$

The main problem in using $\|\hat{U}_{1/2}^n - U_1^n\|_1$ as an a posteriori estimate of $\|u - U_1^n\|_1$ is the computational effort required to obtain $\hat{U}_{1/2}^n$. This cost can be reduced considerably by using the superconvergence property of the finite element method for one-dimensional parabolic systems. Nodal superconvergence enables us to approximate $\hat{U}_{1/2}^n$ as

$$\hat{U}^n_{1/2} = U^n_{1/2} + E^n_{1/2} \qquad (6)$$

where $E^n_{1/2}$ is a "hierarchical" correction term obtained by trapezoidal rule integration and piecewise quadratic finite elements which vanish at the nodes.

As described above,

$$\bar{e}^n := \|U^n_{1/2} + E^n_{1/2} - U^n_1\|_1 \qquad (7)$$

furnishes an estimate to the error $\|u - U^n_1\|_1$ of the backward Euler solution. Equation (7) suggests the inequality

$$\bar{e}^n \leq \|U^n_{1/2} - U^n_1\|_1 + \|E^n_{1/2}\|_1 \ . \qquad (8)$$

The term $\|U^n_{1/2} - U^n_1\|_1$ is the difference between two piecewise linear solutions computed with temporal integration schemes of different orders and can be regarded as a measure of the temporal discretization error. In a similar manner, $\|E^n_{1/2}\|_1$ can be regarded as a measure of the spatial discretization error. Indeed, when the finite element system is integrated exactly in time, Adjerid and Flaherty (ref 1) proved that $\|E\|_1$ converges to the exact spatial discretization error $\|u - U\|_1$ as $N \rightarrow \infty$ for linear parabolic problems.

The refinement algorithm utilizing the above error estimates is described in detail in the next section. Following that, we describe how error estimates are used to determine the necessary level of refinement. Finally, a summary of this report is presented.

MESH REFINEMENT ALGORITHM

The error estimates discussed in the previous section are used to control a global mesh refinement procedure that maintains $\bar{e}^n$ (cf., Eq. (7)) below a specified tolerance TOL. Suppose that a solution U^{n-1}_1, and error estimates $E^{n-1}_{1/2}$ and $\bar{e}^{n-1}$ have been calculated at time t^{n-1} using a mesh with N elements and time step Δt^{n-1}. Further suppose that $\bar{e}^{n-1} <$ TOL and calculate solutions and error estimates at time $t^n = t^{n-1} + \Delta t^n$ using a mesh with N elements and time step $\Delta t^n = \Delta t^{n-1}$. The refinement strategy consists of checking $\bar{e}^n$ and proceeding as follows:

1. If $\bar{e}^n \leq \|U^n_{1/2} - U^n_1\|_1 + \|E^n_{1/2}\|_1 \leq$ TOL, continue to the next time step.

2. If $\bar{e}^n >$ TOL, $\|U^n_{1/2} - U^n_1\|_1 \geq$ ½ TOL and $\|E^n_{1/2}\|_1 \geq$ ½ TOL, then determine a new Δt^n and a new N, and redo the integration. (The procedure for determining the new Δt^n and N are illustrated in the next section.)

3. If $\bar{e}^n >$ TOL, $\|U^n_{1/2} - U^n_1\|_1 <$ ½ TOL and $\|E^n_{1/2}\|_1 \geq$ ½ TOL, then determine a new N and redo the integration.

4. If $\bar{e}^n$ > TOL, $\|U^n_{1/2} - U^n_1\|_1 \geq$ ½ TOL and $\|E^n_{1/2}\|_1 <$ ½ TOL, then determine a new Δt^n and redo the integration.

Steps 2 through 4 are repeated until step 1 is satisfied. If the new Δt^n and/or N are properly determined, however, no additional repetition should be necessary. The choice of ½ TOL was determined as the most efficient from various numerical experiments.

The main advantage of this refinement procedure is that separate estimates of the spatial and temporal errors allow different strategies to be used depending upon the dominant component of the error. Thus, if the spatial component of the error, as measured by $\|E^n_{1/2}\|$ is large, then only spatial refinement is used to reduce the total error. The opposite situation arises when the spatial component of the error is small relative to the temporal component.

It is important to note that the error estimates used in this refinement procedure are, at best, only asymptotically correct. Thus, they will not produce reliable estimates on coarse meshes or when errors are large. However, these estimates should still indicate when refinement is needed and how to perform it (cf., Adjerid and Flaherty (ref 1) and Moore and Flaherty (ref 8)).

A local refinement strategy, such as those considered in Berger and Oliger (ref 5) and Moore and Flaherty (ref 8), is usually more efficient than the local/global strategy presented herein. The plan here is to combine refinement with a mesh moving method that equidistributes the change of some local error measure for a single time step on a mesh with a fixed number of finite elements (cf., Coyle (ref 38) and Coyle and Flaherty (ref 31)). It may be possible to use this local/global refinement strategy in conjunction with such a mesh moving method since the change in the local error measure will be approximately the same on every subinterval.

REFINEMENT DETERMINATION

The choices for the spatial and temporal refinement levels are made simply and straightforwardly and without undue computational effort. Yet these choices try to take advantage of the error estimators already computed and the known asymptotic nature of the true error.

The choice of a new time step, Δt^n, is simple with global temporal refinement. Since the local temporal error of the Backward Euler Method is $O(\Delta t^2)$, it may be reduced by a factor of r, $0 < r < 1$, by reducing Δt by a factor of $r^{1/2}$. Let $E(\Delta t)$ denote the temporal error for a time step, Δt. If the temporal error is such that $E(\Delta t^{n-1})$ > ½ TOL, then one needs to reduce the error by some factor less than

$$\gamma = \frac{\frac{1}{2}\, TOL}{E(\Delta t^{n-1})}\ ; \qquad \textbf{(9)}$$

thus, a reasonable choice for r is $\frac{3}{4}\gamma$. This results in a choice for Δt^n such that

$$\Delta t^{n} = r^{\frac{1}{2}} \Delta t^{n-1} = \sqrt{\frac{(0.75)\frac{1}{2}TOL}{E(\Delta t^{n-1})}}\,\Delta t^{n-1} . \tag{10}$$

Let $E(x,t)$ denote the pointwise spatial error function at time t, then our objective is

$$\left[\int_a^b E^2(x,t)dx\right]^{\frac{1}{2}} < \tfrac{1}{2}\,TOL . \tag{11}$$

Rewriting Eq. (11) in terms of the underlying spatial discretization yields

$$\left[\sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} E^2(x,t)dx\right]^{\frac{1}{2}} < \tfrac{1}{2}\,TOL . \tag{12}$$

Equation (12) implies a finer discretization is needed in the interval (x_{j-1},x_j) if

$$\int_{x_{j-1}}^{x_j} E^2(x,t)dx > \frac{\frac{1}{4}TOL^2}{N} = TOL_1 . \tag{13}$$

Furthermore, since the true spatial error on (x_{j-1},x_j) for piecewise linear elements is such that (cf., Wendroff (ref 39))

$$\int_{x_{j-1}}^{x_j} E^2(x,t)dx \sim \left(\frac{x_j - x_{j-1}}{N_j}\right)^2 , \tag{14}$$

where N_j is the number of elements into which (x_{j-1},x_j) is subdivided, then to reduce the spatial error by a factor of r, one should add $r^{-\frac{1}{2}}$ elements to (x_{j-1},x_j). This leads to a choice of N_j such that

$$r^{-\frac{1}{2}} = \left[\frac{TOL_1}{\int_{x_{j-1}}^{x_j} E^2(x,t)\,dx}\right]^{\frac{1}{2}} < N_j \tag{15}$$

Picking N_j such that

$$N_j = floor\left(r^{-\frac{1}{2}}\right) + 1 \tag{16}$$

will ensure that N_j satisfies Eq. (15).

Example 1

Consider the following problem for Burgers' equation:

$$u_t + uu_x = \epsilon u_{xx} \ , \ 0 < x < 1 \ , \ t > 0 \ , \tag{17a}$$

$$u(x,0) = \sin \pi x \ , \ u(0,t) = u(1,t) = 0 \ , \tag{17b,c,d}$$

where $\epsilon = 5\times10^{-3}$. The solution of this problem is a pulse that steepens as it travels to the right until it forms a shock layer at $x = 1$. After a time of $O(\epsilon^{-1})$, the pulse dissipates and the solution decays to zero (cf. Figure 1, at the end of this section).

This problem was solved for a value of TOL equal to 0.8 but with different initial values for N and Δt. In Table 1, a summary of the results is presented when N and Δt are initially 100 and 0.1, respectively. Table 2 presents a summary for when N is initially 20 and Δt is initially 0.02. Table 3 summarizes results when N and Δt are initially 50 and 0.1. Mesh trajectories corresponding to the data presented in Tables 1, 2, and 3 are shown in Figures 2, 3, and 4, respectively (at the end of this section). The horizontal lines in these figures are used to distinguish the regions where the values of Δt are different.

These tables present the relevant refinement data for the significant time levels of the solution process. By a "significant time level," we mean a time level at which a refinement has occurred and one immediately preceding a refinement. The tables are divided into four columns labelled "Significant Times," "N" (with the initial N in parentheses), "Δt" (with the initial Δt in parentheses), and "Error Estimate," respectively. The significant time levels are found in the first column. Reading across the tables, one finds the values of N and Δt necessary to complete the solution step to within the given tolerance. A dash is used to indicate no change in N or Δt from the preceding row. The last column lists the value of $\bar{e}^n$ at the successful completion of the time step. The last row of each table contains results for the final time of 0.8. In this manner, the tables outline the refinement process giving some indication as to why refinement occurred, as well as demonstrating the success of the process.

These results indicate that it is possible to reduce the total error by refining only in space or only in time, and that the error estimates $\bar{e}^n$, $\|U^n_{1/2} - U^n_1\|_1$, and $\|E^n_{1/2}\|_1$ can be used to detect when these situations arise.

Table 1 **Numerical Parameters For Solving Example 1 With TOL = 0.8 and N and Δt Initially 100 and 0.1, Respectively**

Significant Times	N (100)	Δt (0.1)	Error Estimate
0.1000	-	-	0.3221
0.1566	-	0.0566	0.2218
0.2131	-	-	0.5436
0.2549	165	0.0417	0.3455
0.8000	-	-	0.2728

Table 2 **Numerical Parameters For Solving Example 1 With TOL = 0.8 and N and Δt Initially 20 and 0.02, Respectively**

Significant Times	N (20)	Δt (0.02)	Error Estimate
0.24	-	-	0.6741
0.26	46	-	0.3710
0.28	-	-	0.4330
0.30	66	-	0.3072
0.38	-	-	0.6210
0.40	109	-	0.2488
0.80	-	-	0.1595

Table 3 **Numerical Parameters For Solving Example 1 With TOL = 0.8 and N and Δt Initially 50 and 0.1, Respectively**

Significant Times	N (50)	Δt (0.1)	Error Estimate
0.1000	-	-	0.3263
0.1573	62	0.0573	0.2227
0.2147	-	-	0.4766
0.2566	81	0.0419	0.3913
0.3405	-	-	0.4662
0.3824	118	-	0.3448
0.8000	-	-	0.1644

BURGER'S EQUATION

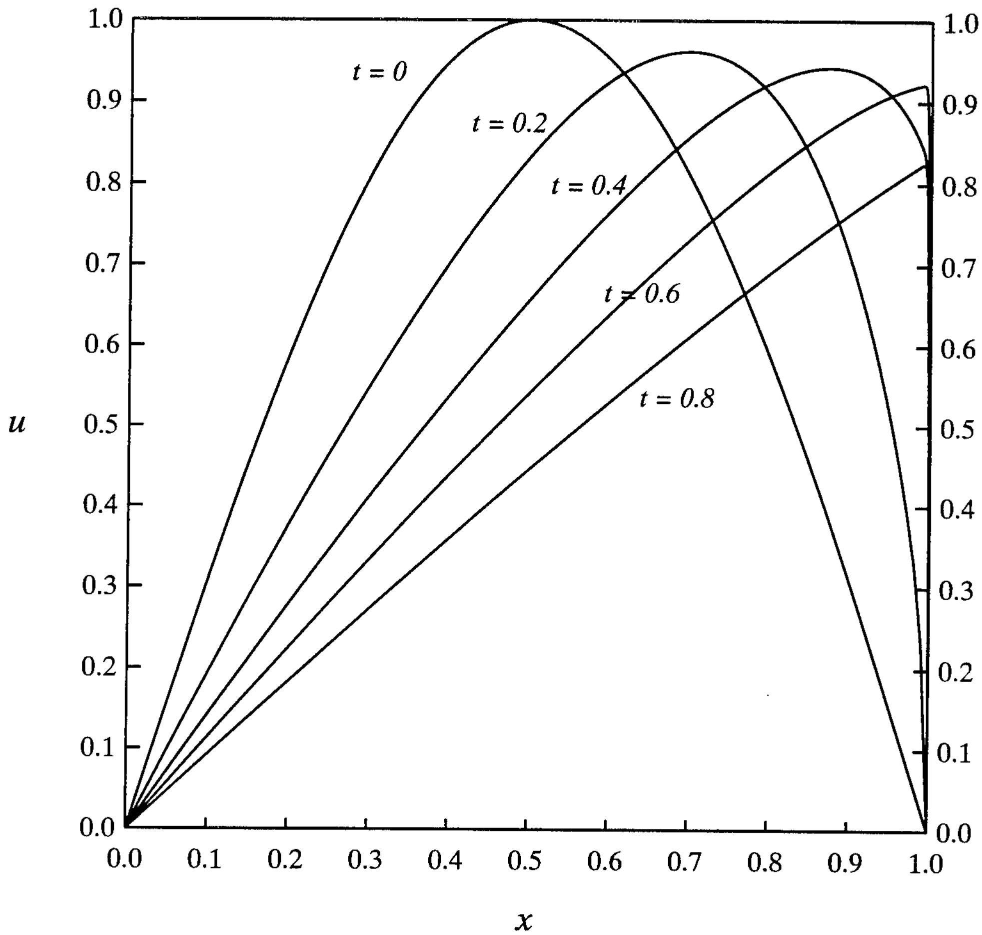

Figure 1. Solutions to Example 1 for several instances of time.

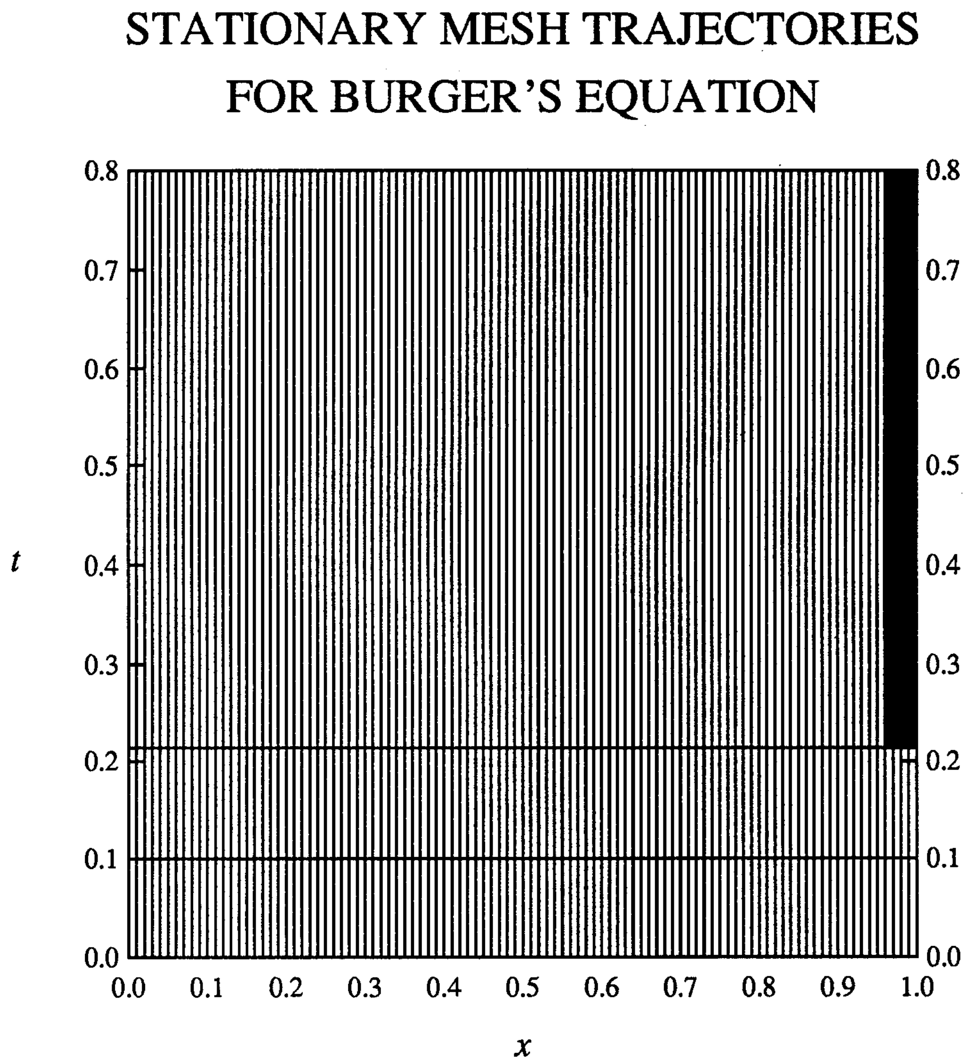

Figure 2. Mesh trajectories for Example 1 corresponding to Table 1.

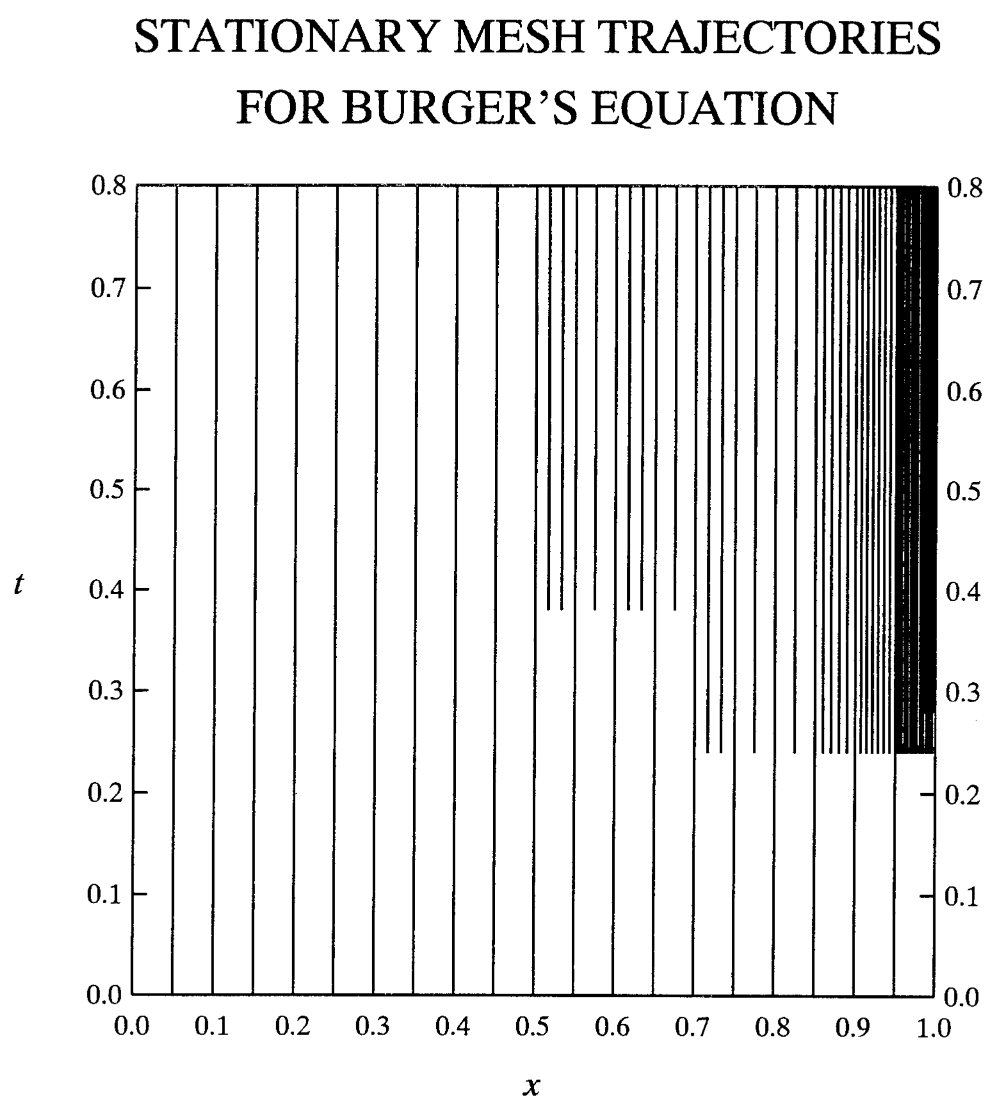

Figure 3. Mesh trajectories for Example 1 corresponding to Table 2.

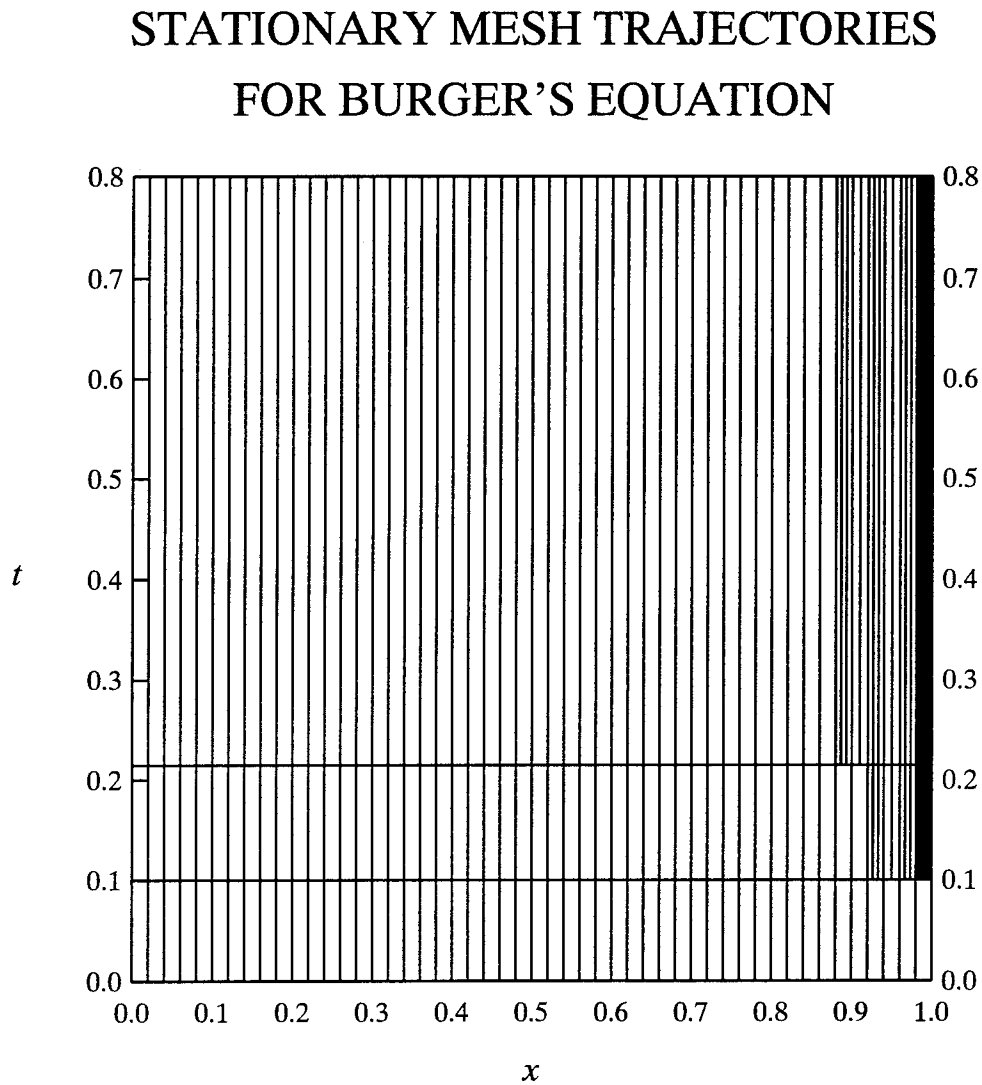

Figure 4. Mesh trajectories for Example 1 corresponding to Table 3.

SUMMARY

The three error estimates in the first section were used to control a global refinement procedure that attempts to maintain a global measure of the error per time step below a prescribed tolerance. Refinement can be performed in space, time, or both space and time depending on the dominant component of the error estimate.

The refinement algorithm consisted of first determining the three error estimates and then comparing them to the given tolerance. If the total error estimate was small enough, no refinement is performed. However, if the total error estimate is large, its spatial and temporal components are checked to see if one is more dominant. If one component dominates, then refinement is performed only in the corresponding dimension. Otherwise, refinement is performed in both space and time.

The magnitude of the refinement is determined automatically, and a means of doing this is presented. This determination is based on a priori estimates of the numerical methods employed.

Finally, Burgers' equation was solved for several initial values for the temporal and spatial discretizations in order to illustrate the refinement algorithm in conjunction with the various error estimates.

The results of Example 1 provide an indication of the utility of these estimates and of this refinement procedure. In certain situations, only spatial and temporal refinement were needed to keep the total error within the prescribed tolerance, and our error estimates could be used to determine when these situations arise.

This is one of the first attempts to simultaneously address spatial and temporal errors with different refinement strategies. Most researchers (cf., e.g., Berger and Oliger (ref 5)) have used binary refinement in space and time, but did not attempt to determine the dominant component of the total discretization error. As noted, method of lines techniques (cf., e.g., Adjerid and Flaherty (ref 1) and Bieterman and Babuska (refs 6,7)) typically assume that temporal integration is exact and refine based on estimates of spatial errors. There is a great potential for techniques that utilize different spatial and temporal refinement strategies, particularly with problems having singularities.

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